

10/542870

=> s l11

SAMPLE SEARCH INITIATED 15:30:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1 TO 80
PROJECTED ANSWERS: 1 TO 80

L12 1 SEA SSS SAM L11

=> s l11 sss ful

FULL SEARCH INITIATED 15:30:48 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 31 TO ITERATE

100.0% PROCESSED 31 ITERATIONS 10 ANSWERS
SEARCH TIME: 00.00.01

L13 10 SEA SSS FUL L11

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	166.94	762.49

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-36.00

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FILE COVERS 1907 - 4 Mar 2006 VOL 144 ISS 11
FILE LAST UPDATED: 3 Mar 2006 (20060303/ED)

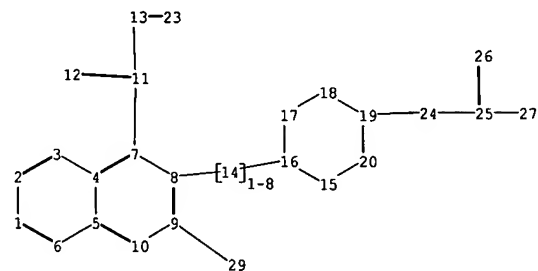
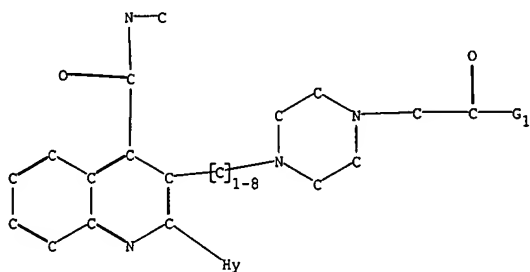
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=> s l13

L14 1 L13

=> d l14 bib abs hitstr



chain nodes :

11 12 13 14 23 24 25 26 27 29

ring nodes :

1 2 3 4 5 6 7 8 9 10 15 16 17 18 19 20

chain bonds :

7-11 8-14 9-29 11-12 11-13 13-23 14-16 19-24 24-25 25-26 25-27

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10 15-16 15-20 16-17 17-18
18-19 19-20

exact/norm bonds :

9-29 11-12 11-13 13-23 14-16 15-16 15-20 16-17 17-18 18-19 19-20 19-24 25-26
25-27

exact bonds :

7-11 8-14 24-25

normalized bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10

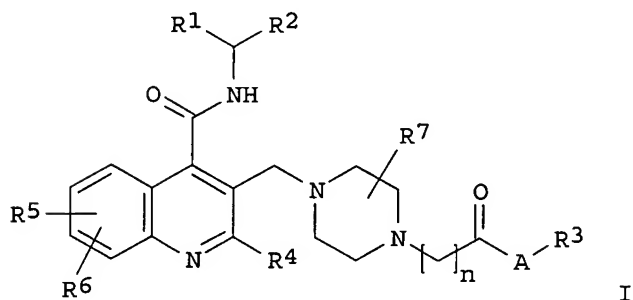
G1:O,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 29:Atom

L14 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2004:648345 CAPLUS
 DN 141:190803
 TI Preparation of quinoline derivatives as NK-2 and NK-3 receptor antagonists
 IN Kerns, Jeffrey; Jin, Qi; Wan, Zehong; Nie, Hong; Zhu, Chongjie
 PA Smithkline Beecham Corporation, USA
 SO PCT Int. Appl., 53 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004066950	A2	20040812	WO 2004-US2366	20040129
	WO 2004066950	A3	20041104		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI			
	EP 1601360	A2	20051207	EP 2004-706434	20040129
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
PRAI	US 2003-443650P	P	20030130		
	WO 2004-US2366	W	20040129		
OS	MARPAT 141:190803				
GI					



AB The title compds. [I; R1 = H, (un)substituted alkyl; R2 = (un)substituted aryl, cycloalkyl, heterocyclyl; R3 = H, (un)substituted alkyl, cycloalkyl, aryl, heterocyclyl; A = NR8, O (R8 = H, (un)substituted alkyl); R4 = (un)substituted heterocyclyl; R5 = H, alkyl, alkenyl, aryl, etc.; or R5 represents a bridging moiety which is arranged to bridge two adjacent ring atoms, wherein the bridging moiety comprises alkylene or dioxyalkylene; R6 = H, halo; R7 = oxo; n = 1-4] which are NK2 and NK3 receptor antagonists and are useful in the treatment of respiratory diseases, were prepd. E.g., a 4-step synthesis of 3-(4-dimethylcarbamoylmethyl-3-oxopiperazin-1-ylmethyl)-2-(thiophen-2-yl)quinoline-4-carboxylic acid [(S)-1-cyclohexylethyl]amide, was given. The most potent compds. I show IC50 in the range 10-1000 nM against NK-3 receptor binding, and IC50 in the range 1-1000 nM against NK-2 receptor binding. The pharmaceutical compn. comprising the compd. I is claimed.

IT 737804-27-2P 737804-30-7P 737804-36-3P

10/542870

737804-40-9P 737804-41-0P 737804-42-1P

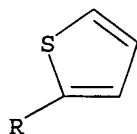
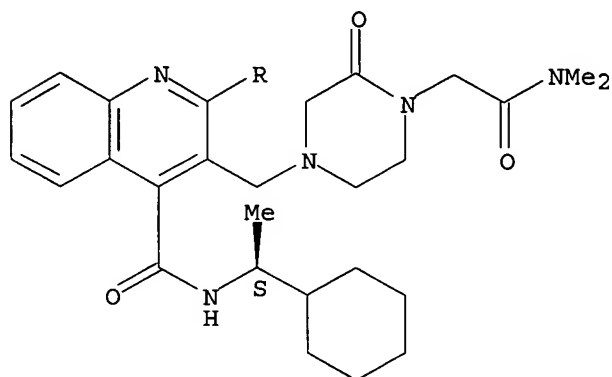
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of quinoline derivs. as NK-2 and NK-3 receptor antagonists for treating respiratory diseases)

RN 737804-27-2 CAPLUS

CN 4-Quinolinecarboxamide, N-[(1S)-1-cyclohexylethyl]-3-[[4-[2-(dimethylamino)-2-oxoethyl]-3-oxo-1-piperazinyl]methyl]-2-(2-thienyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

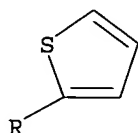
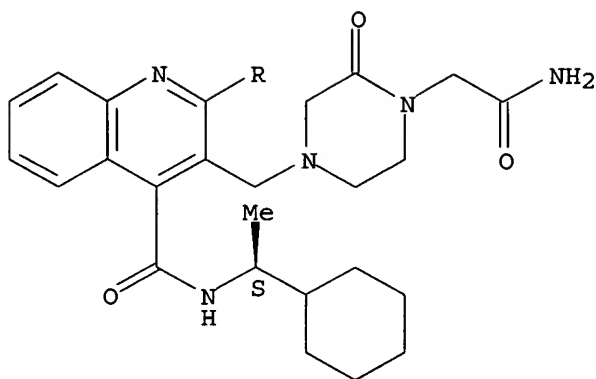


RN 737804-30-7 CAPLUS

CN 4-Quinolinecarboxamide, 3-[[4-(2-amino-2-oxoethyl)-3-oxo-1-piperazinyl]methyl]-N-[(1S)-1-cyclohexylethyl]-2-(2-thienyl)-(9CI) (CA INDEX NAME)

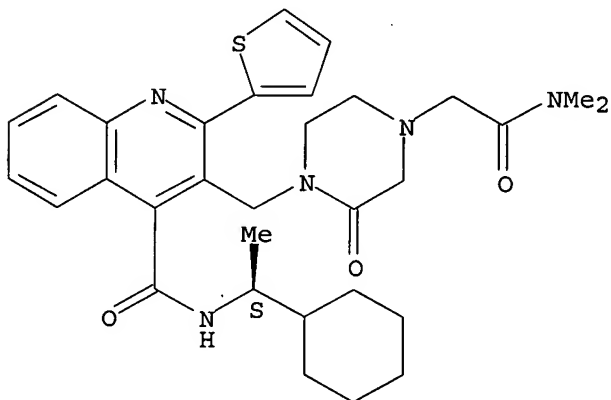
Absolute stereochemistry.

10/542870



RN 737804-36-3 CAPLUS
CN 4-Quinolinecarboxamide, N-[(1S)-1-cyclohexylethyl]-3-[[4-[2-(dimethylamino)-2-oxoethyl]-2-oxo-1-piperazinyl]methyl]-2-(2-thienyl)-(9CI) (CA INDEX NAME)

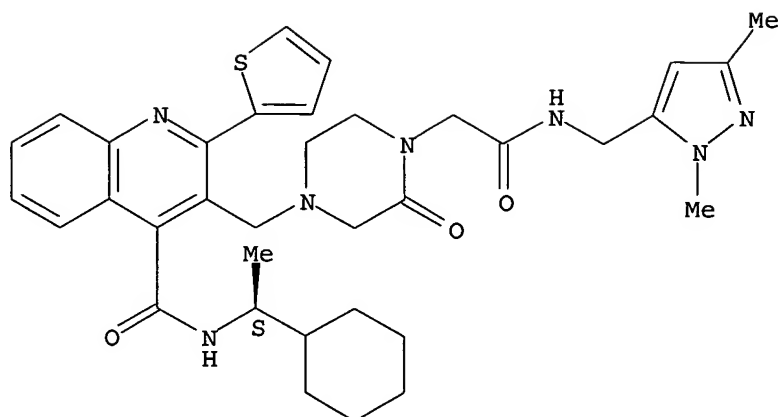
Absolute stereochemistry.



RN 737804-40-9 CAPLUS
CN 4-Quinolinecarboxamide, N-[(1S)-1-cyclohexylethyl]-3-[[4-[2-[[[(1,3-dimethyl-1H-pyrazol-5-yl)methyl]amino]-2-oxoethyl]-3-oxo-1-piperazinyl]methyl]-2-(2-thienyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

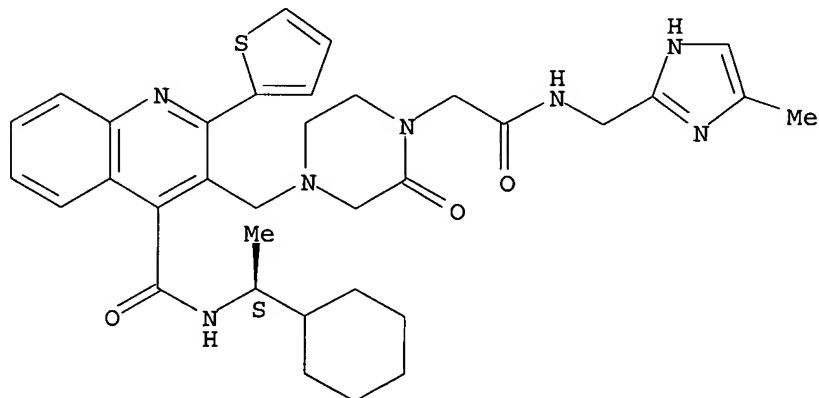
10/542870



RN 737804-41-0 CAPLUS

CN 4-Quinolinecarboxamide, N-[(1S)-1-cyclohexylethyl]-3-[[4-[2-[[4-methyl-1H-imidazol-2-yl)methyl]amino]-2-oxoethyl]-3-oxo-1-piperazinyl]methyl]-2-(2-thienyl)- (9CI) (CA INDEX NAME)

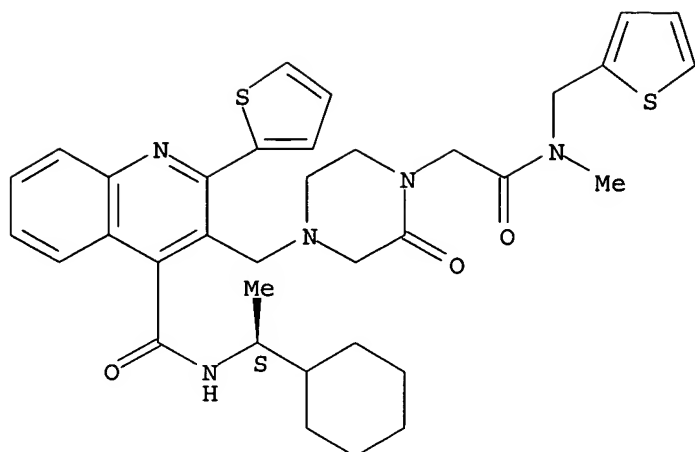
Absolute stereochemistry.



RN 737804-42-1 CAPLUS

CN 4-Quinolinecarboxamide, N-[(1S)-1-cyclohexylethyl]-3-[[4-[2-[methyl(2-thienyl)methyl]amino]-2-oxoethyl]-3-oxo-1-piperazinyl]methyl]-2-(2-thienyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 737804-43-2P 737804-46-5P 737804-47-6P
737804-48-7P

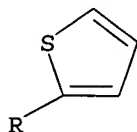
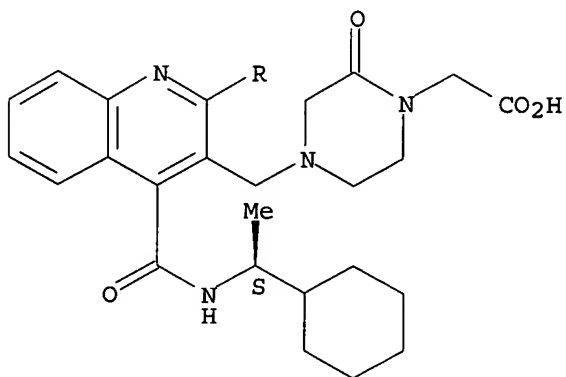
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of quinoline derivs. as NK-2 and NK-3 receptor antagonists for treating respiratory diseases)

RN 737804-43-2 CAPLUS

CN 1-Piperazineacetic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-2-(2-thienyl)-3-quinolinyl]methyl]-2-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

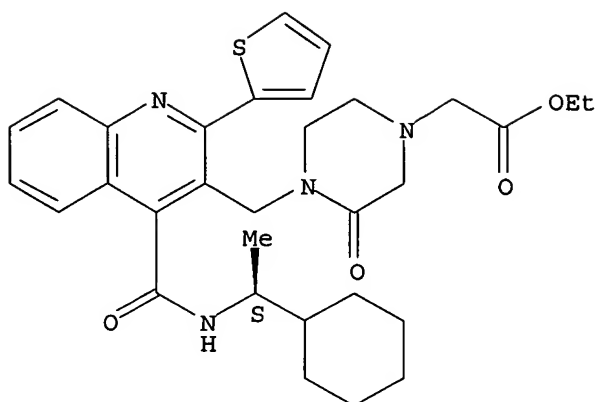


RN 737804-46-5 CAPLUS

CN 1-Piperazineacetic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-2-(2-thienyl)-3-quinolinyl]methyl]-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

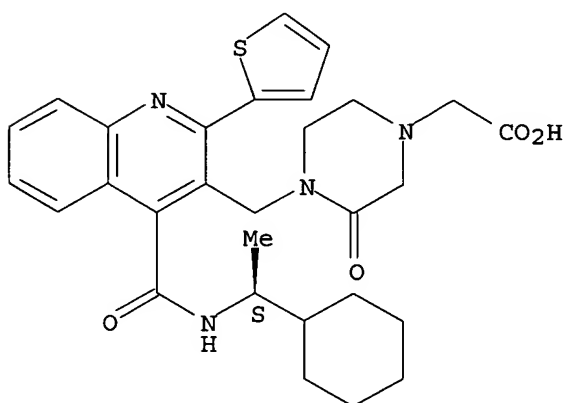
10/542870



RN 737804-47-6 CAPLUS

CN 1-Piperazineacetic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-2-(2-thienyl)-3-quinolinyl]methyl]-3-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

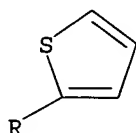
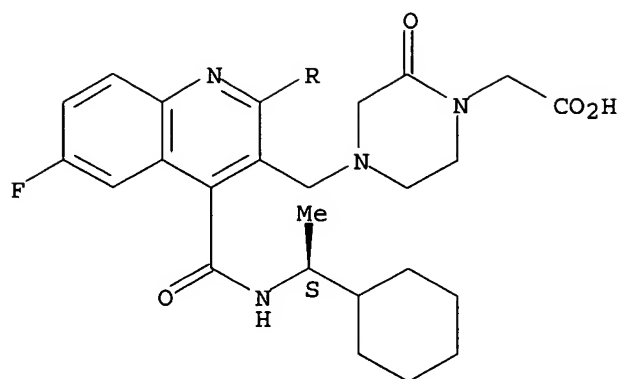


RN 737804-48-7 CAPLUS

CN 1-Piperazineacetic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-6-fluoro-2-(2-thienyl)-3-quinolinyl]methyl]-2-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/542870



=> file caold
COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
5.57	768.06

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.75	-36.75

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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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=> s l13
L15 0 L13

=> log h

10/542870

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.44	768.50
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-36.75

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 15:31:21 ON 04 MAR 2006

EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	1594	((544/121) or (544/357)).CCLS.	US-PGPUB; USPAT	OR	OFF	2006/03/04 21:12
L2	465	NK-2 or NK-3	US-PGPUB; USPAT	OR	OFF	2006/03/04 21:12
L3	8	l1 and l2	US-PGPUB; USPAT	OR	OFF	2006/03/04 21:12